Development of Stress Corrosion Cracking Model for Reactor Structural Materials

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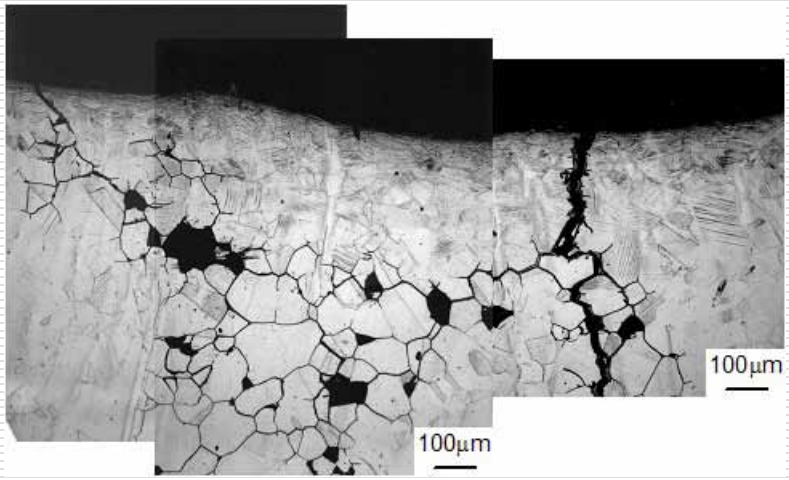
Contents

- Background and objectives
- Macro scale approach
  - 2-D SCC growth model
- Micro scale approach
  - Influences of impurities on bond strength of grain boundary
  - Bond energy analysis of random grain boundary of bcc iron system
  - Interaction between grain boundary and dislocation
- Summary

Background and objectives

Background

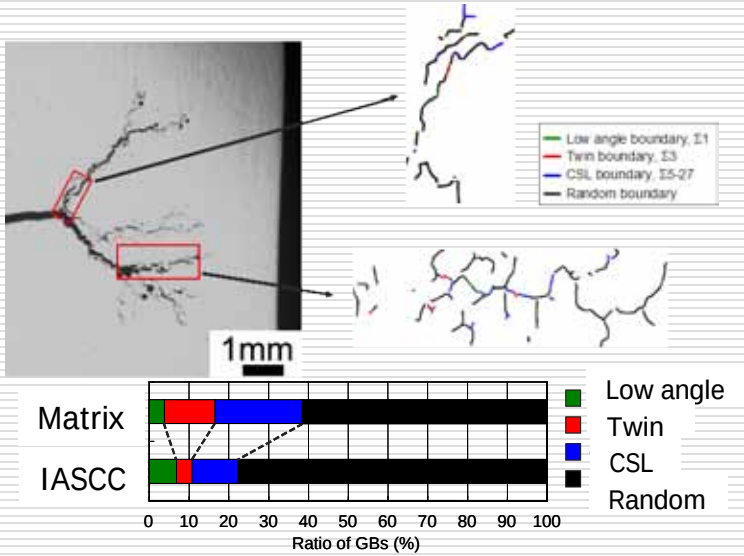
- Stress corrosion cracking (SCC) is one of key issues in aging LWRs.
- **Irradiation assisted stress corrosion cracking (IASCC)** is caused by synergistic effects of neutron radiation, stress/strain and high temperature water on structural materials.
- Important factors on SCC are stress and segregation (corrosion) at grain boundaries, because SCC propagate mainly along random grain boundaries.



SCC at core shroud of boiling water reactor

Objectives

- Development of new intergranular stress corrosion cracking (IGSCC) growth model
- Investigation of mechanism of IGSCC



Grain boundary character map (Experiment)

2-D SCC growth model

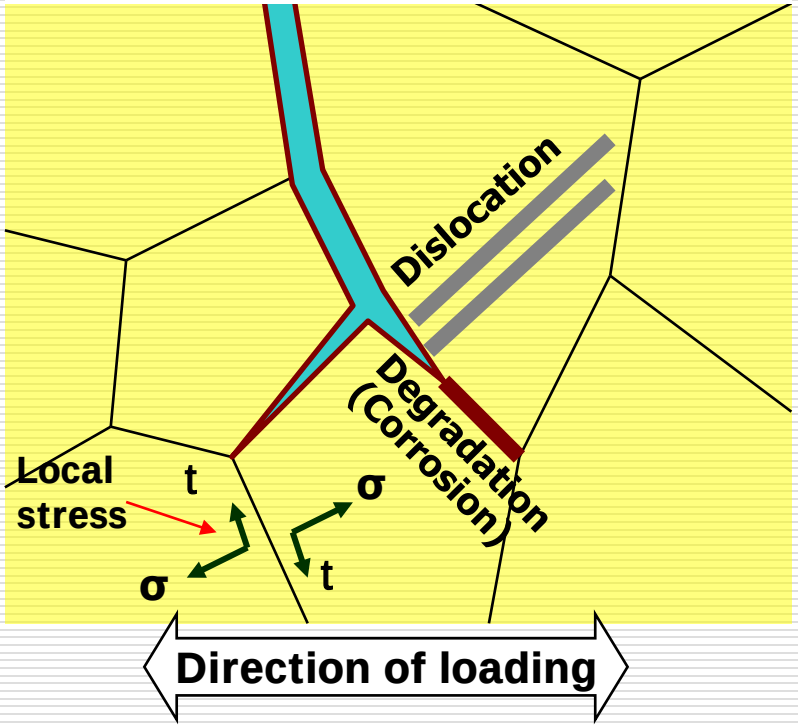
Features of model:

1) Strength of grain boundary

Strength of grain boundary is different with characters of grain boundary, dislocation, …

Face centered cubic (FCC) structure has many slip planes

Variations of strength of grain boundary would become small due to slip dislocation.



Strength of grain boundary with small fluctuation s_{th} is defined as

$$s_{th} = s_0 + fl$$

s_0 : base strength of grain boundary
fl : fluctuation using normal distribution function

2-D SCC growth model

2) Influence of shear stress

… Complex stress constructed by vertical and shear stress is "*locally*" acted on grain boundary around crack tip

"Net stress" h is defined

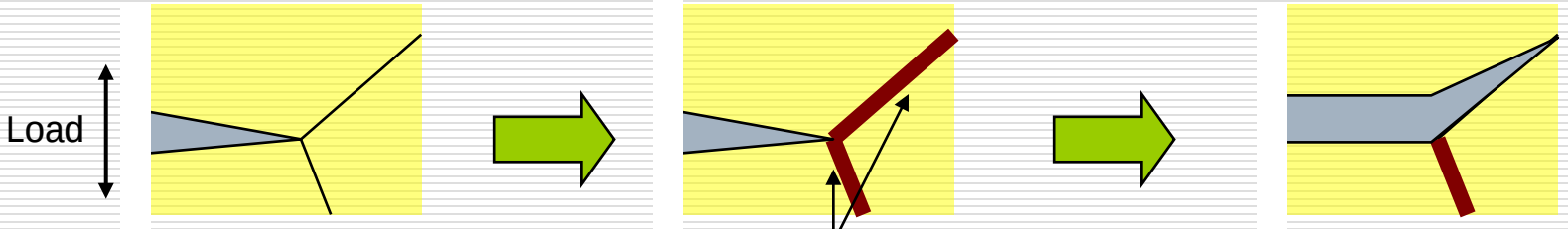
$$h \propto s + at$$

- s : vertical stress against grain boundary
- t : shear stress against grain boundary
- a : parameter to control effect of shear stress

3) Degradation of grain boundary

Assumption :

When stress acted on grain boundary is low, influence of corrosion is dominant relatively to that of stress factor on fracture process.



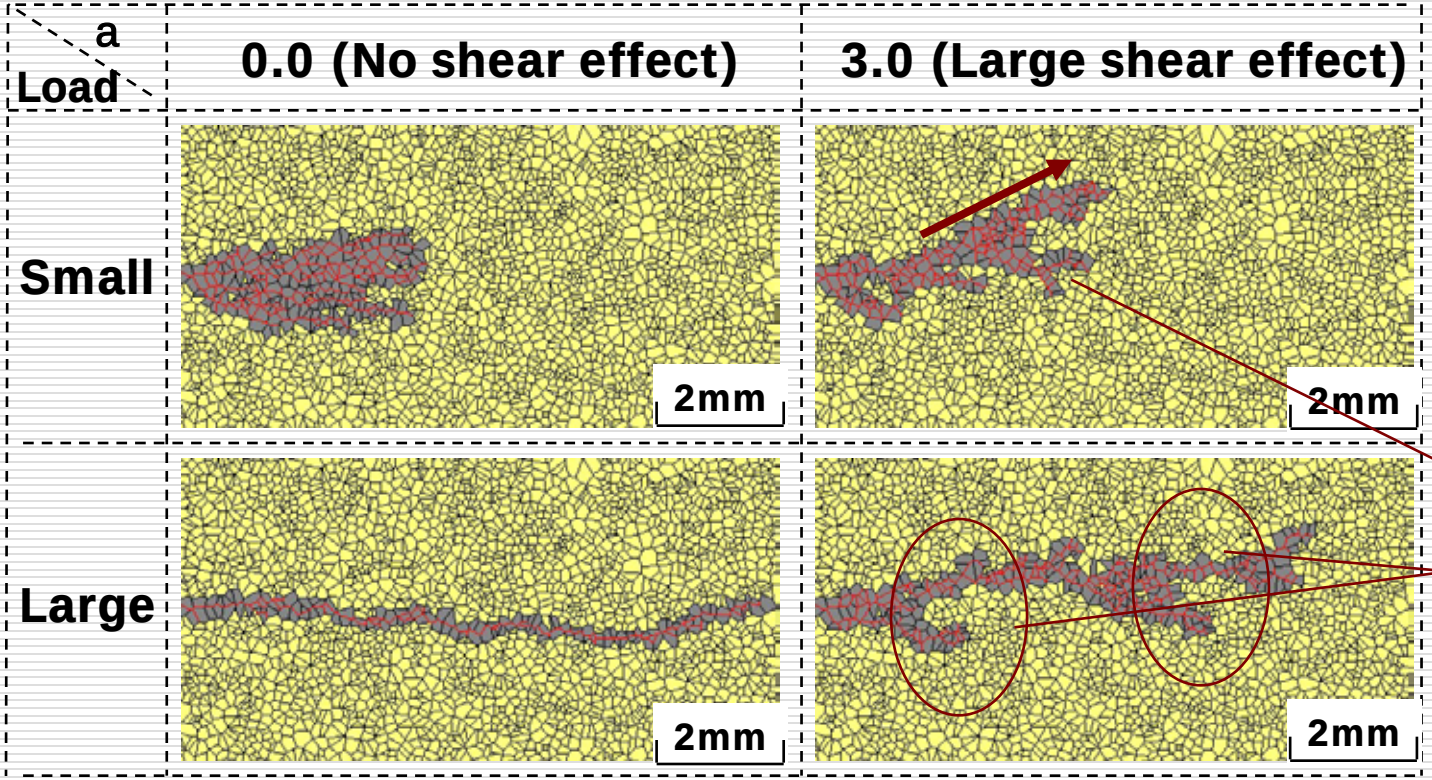
i) Very low load is applied to the system.

ii) Corrosion occurs at grain boundary, and strength weakens.

iii) Crack propagates.

Corrosion is modeled by introducing "slow fracture" of grain boundary.

IGSCC growth analytical results



(T. Igarashi et al., J. Power and Energy System, Vol.2 No.4, pp.1188-1196 (2008))

- **Large load (stress dominant) and a=3.0 : Crack branching**
  - à Main factor of crack branching is effect of shear stress.
- **Small load (corrosion dominant) and a=3.0 : Oblique crack growth**
  - à Synergistic effect of shear stress and corrosion of grain boundary leads to crack growth to oblique direction.

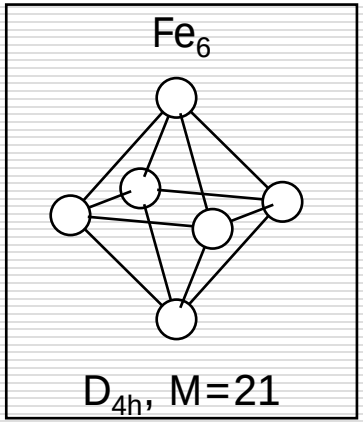
Influences of impurities on bond strength of grain boundary

Computational method:

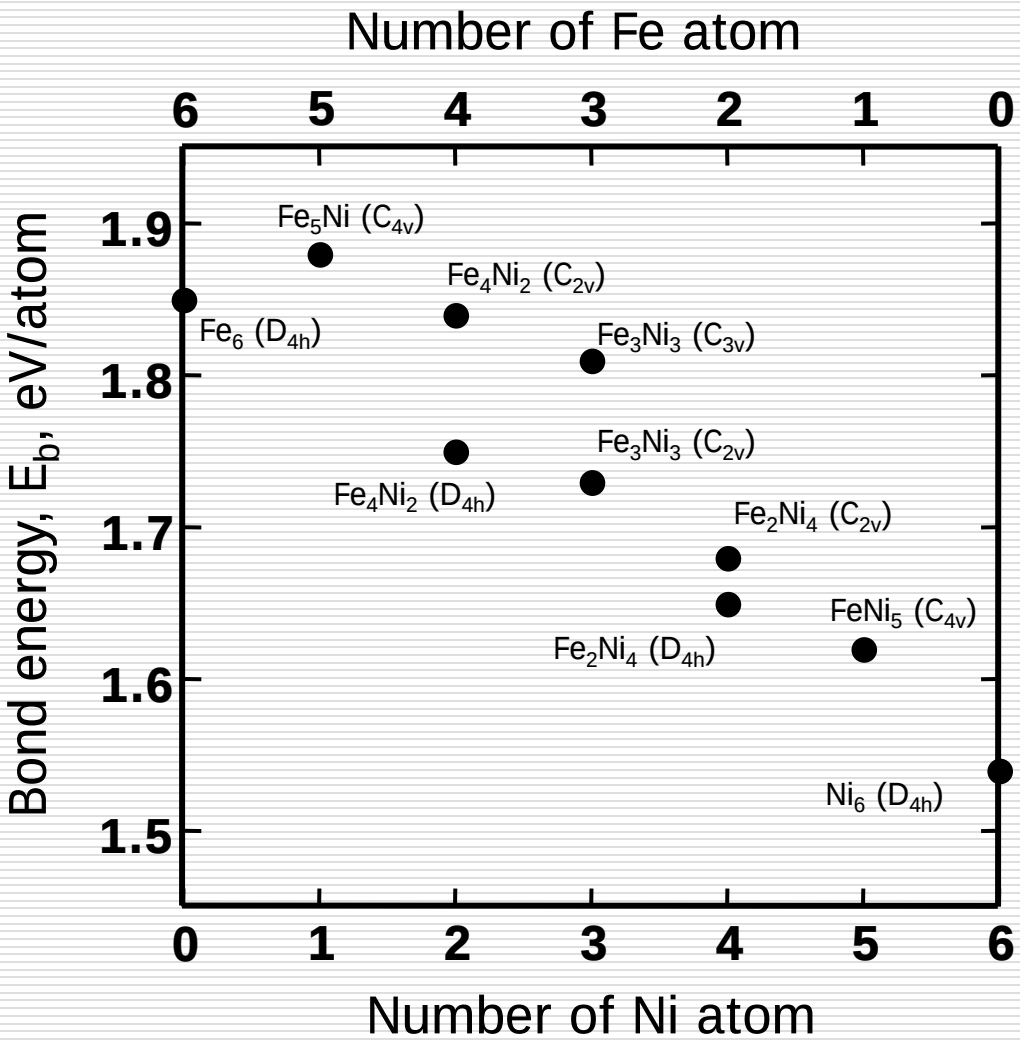
- Theory: Density Functional Theory (DFT)-UB3LYP
- Basis set: LanL2DZ
- Computer program: Gaussian03
- Clusters: $Fe_{6-x}Ni_x$ ($0 \leqq x \leqq 6$), 10 geometries
- Bond energy (E_b)

$$E_b = \frac{E_{cluster} - (n - x)E^{at}_{Fe} - xE^{at}_{Ni}}{n}$$

$E_{cluster}$: energy of alloy cluster, E^{at}_{Fe}: energy of iron atom with M=5, E^{at}_{Ni}: energy of nickel atom with M=3, M: spin multiplicities.



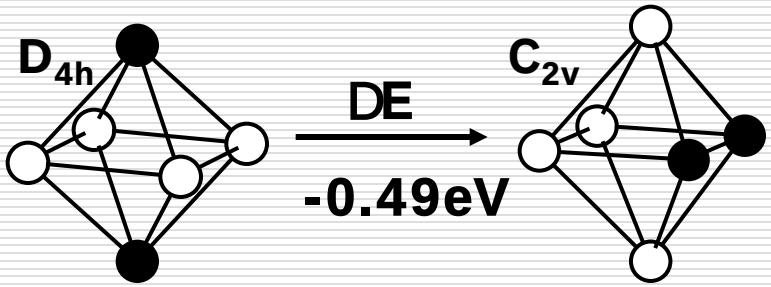
Bond energies of $Fe_{6-x}Ni_x$



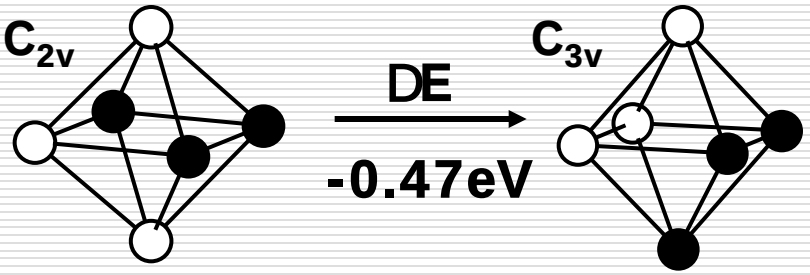
Comparisons on total energies of isomers for Ni substituted Fe_6 clusters

(○: Fe, ●: Ni)

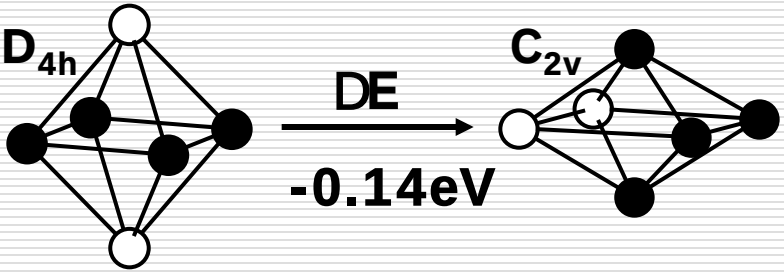
Fe_4Ni_2



Fe_3Ni_3



Fe_2Ni_4



- Ni atoms energetically prefer clustering in the mixed Fe-Ni clusters.
- Clustering leads to a segregation of Ni atoms from Fe atoms.

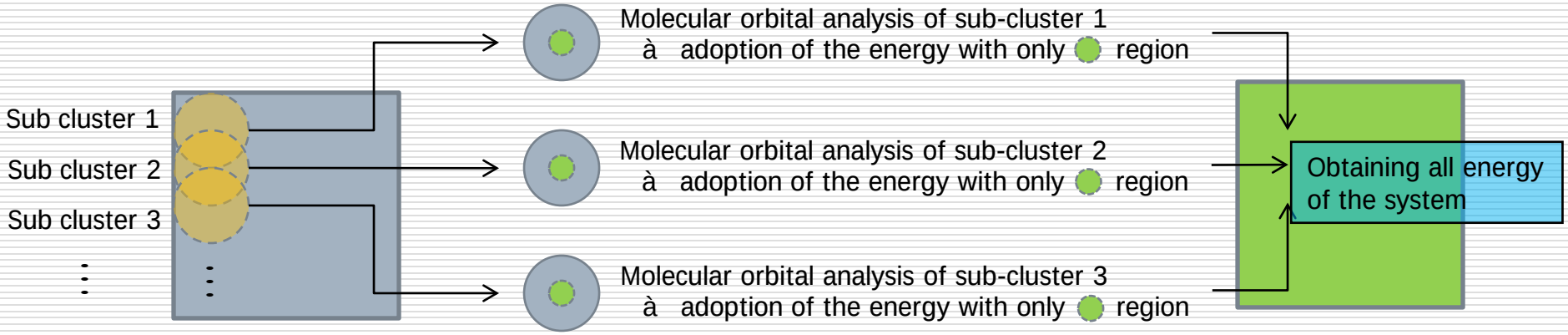
Bond energy analysis of random grain boundary of bcc iron system

Extended semi-empirical molecular orbital method:

I. semi-empirical molecular orbital method with PM6 Hamiltonian

- Faster calculation than ab initio method
- Applicable to all main group and transition metals

II. Partitioning the system into sub-cluster

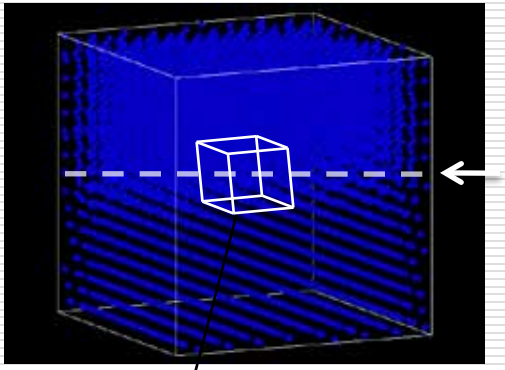


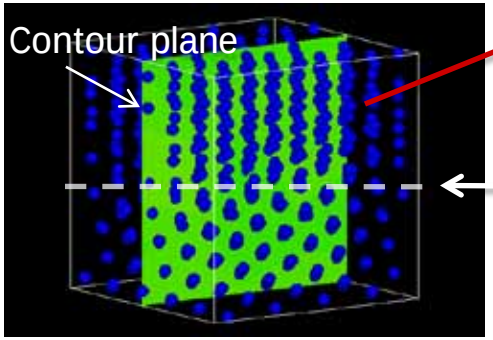
Schematic view of Partitioning the system into sub-cluster

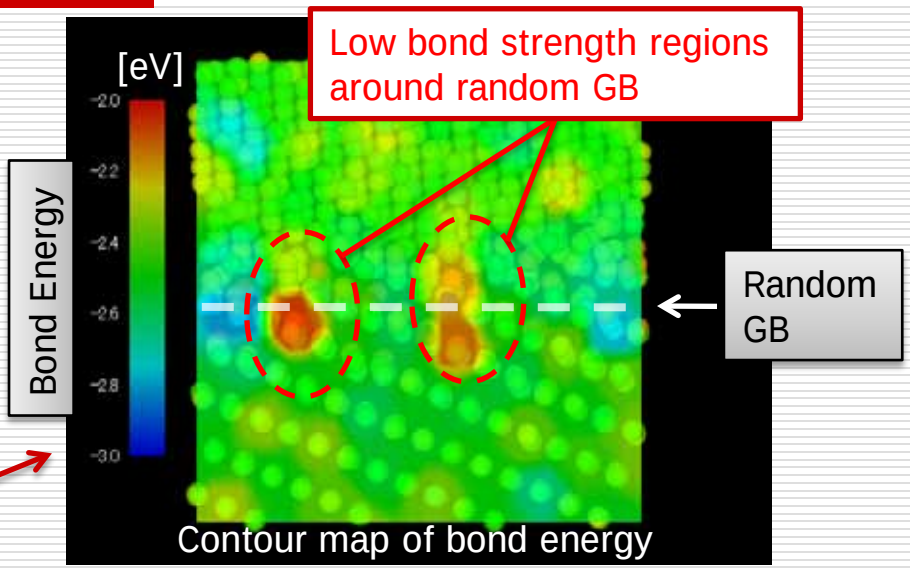
Quantum analysis of large scale alloy system includes ~10^4 atoms such as random grain boundary system of stainless steel.

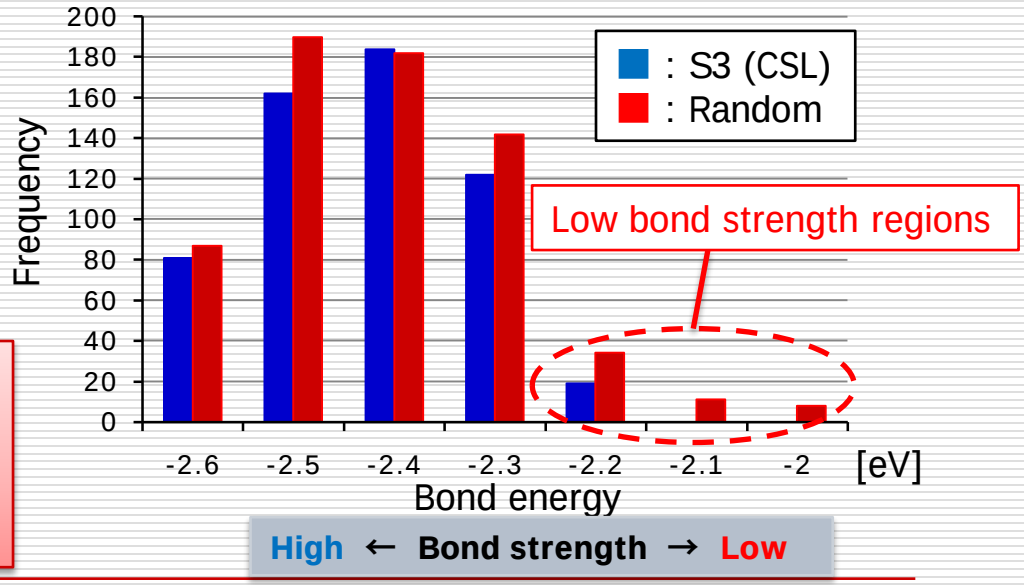
Bond energy of random grain boundary of bcc iron system

Number of atoms : 5346
Radius of sub-cluster sphere : 3.5 Å









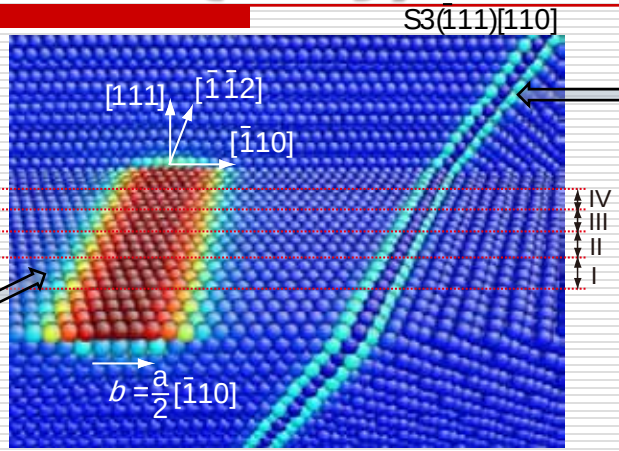
Low bond strength regions appear around random GB as compared with CSL GB.
→ Cause that SCC mainly propagate along random grain boundaries

Interaction between GB and dislocation (Al S3<110>{111})

Computational method:

Atomistic transition state analysis (nudged elastic band (NEB) method)

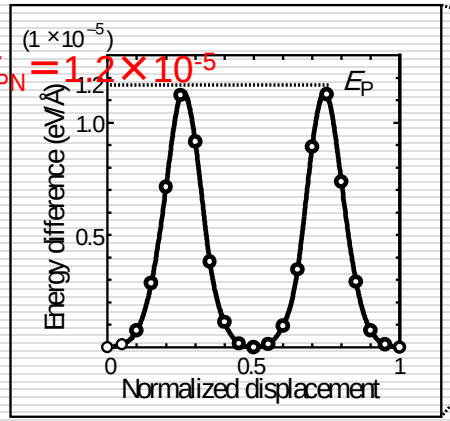
A pure edge dislocation

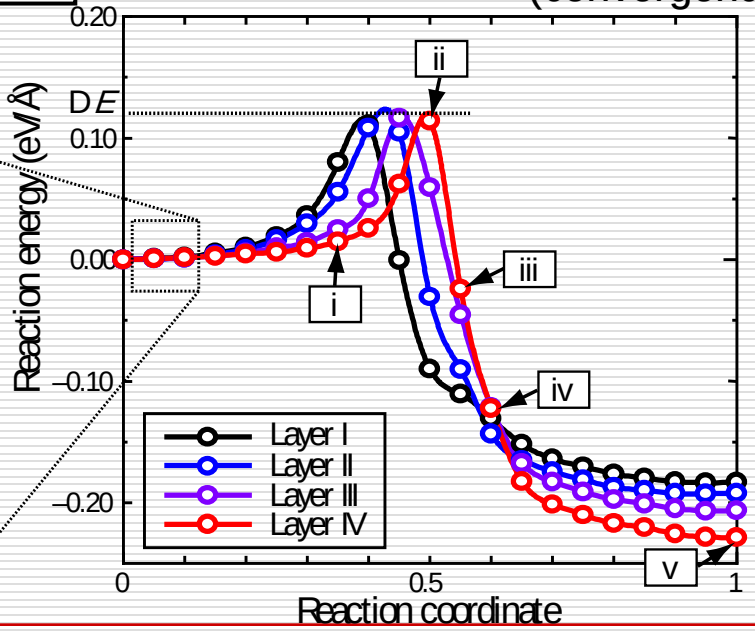


Most stable S3 grain boundary

MEP of interaction process

NEB analysis
(convergence condition=0.01eV/Å)





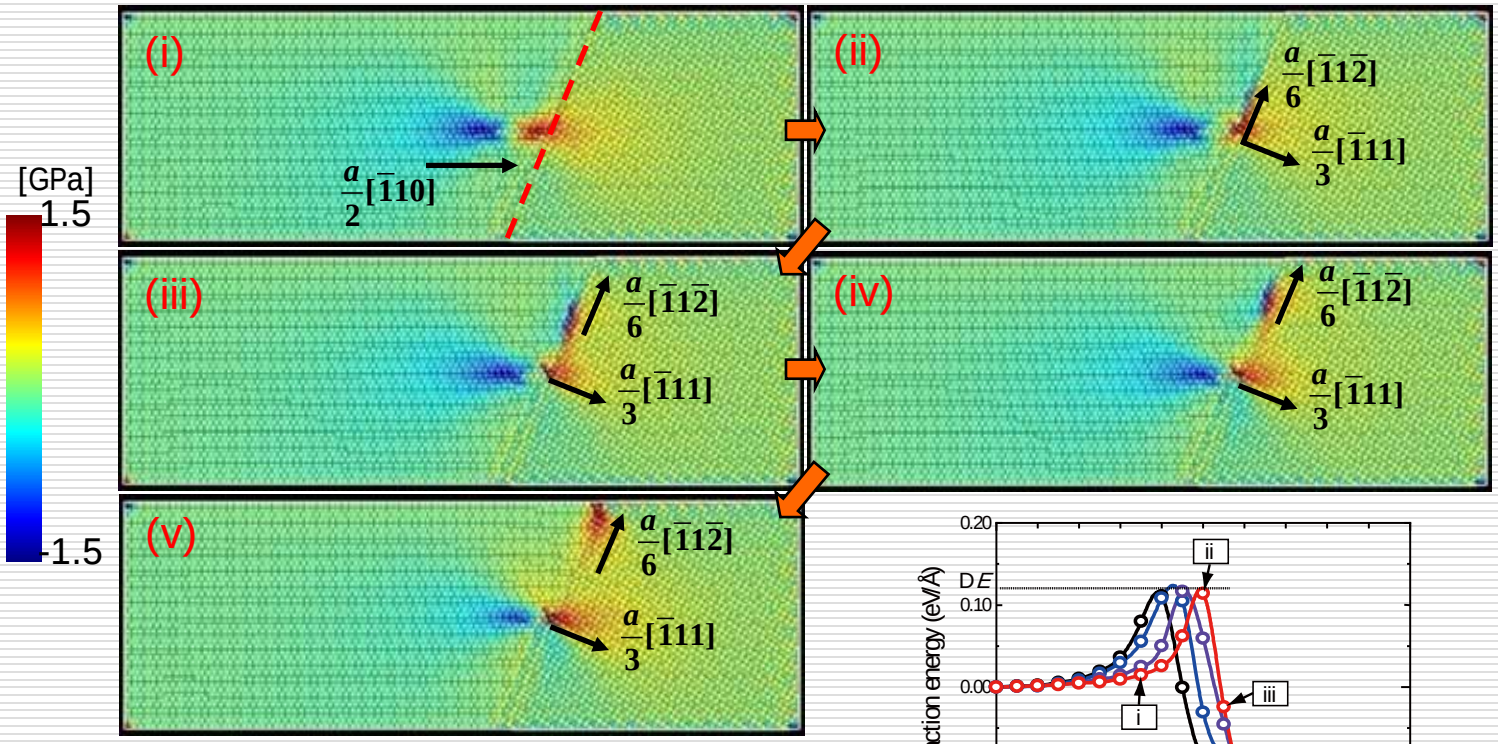
DE = 1.16×10^{-1} [eV/Å]

Peierls potential:
E_{PN}=1.2×10^{-5} [eV/Å]

Effect on plastic deformation (acting as a high energy barrier)

Mechanism of interaction between GB and dislocation (Al S3<110>/{111})

Distribution of t_{zx}



On S3 GB plane: *Resolving at interface*

$$\frac{a}{2}[\bar{1}10] \rightarrow \underbrace{\frac{a}{6}[\bar{1}\bar{1}2]}_{\text{DSC Lattice}} + \underbrace{\frac{a}{3}[\bar{1}11]}_{\text{Step dislocation}}$$

(T. Tsuru et al., APCOM '07-EPMESC XI (2007))

Summary

We have developed IGSCC growth model by multi-scale approach in order to investigate mechanism of SCC and predict SCC behavior. Results of fundamental research activities are as follows;

- Two dimensional IGSCC growth model has been developed and confirmed effect of shear stress and corrosion on grain boundaries for crack branching.
- Bond energies of Fe_m clusters decrease with increasing number of Ni atoms in ab initio calculation.
- Low bond strength regions appear around random grain boundary as compared with S3 grain boundary in bond energy analysis of random grain boundary of bcc iron system.
- Interaction between S3 grain boundary and edge dislocation was investigated by atomistic transition state analysis.